University of California San Diego
9500 Gilman Drive
La Jolla, CA 92093-0736

September 19, 2016

Dear Drs. Mobley and Chodera:

We write to confirm our enthusiastic support of your proposal, “Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations”, and to confirm our willingness to collaborate on the blind challenges you propose.

As Co-Directors of the NIH-funded Drug Design Data Resource (D3R), we work with the pharmaceutical industry and academic labs to obtain high-quality protein-ligand binding data, and we use these data as the basis for blinded prediction challenges that test and drive improvement in methods for pose prediction and affinity calculation. These challenges are informative, as they test the full computational workflow, including preparation of the protein and ligand structures, assignment of protonation states, assignment of force field parameters, and conformational searching and sampling. By the same token, however, they are limited in their ability to assess which aspect of the calculations are the most in need of improvement. Your plan to develop new datasets for simple, model systems, and to use them to continue the SAMPL series of blinded prediction challenges, is strongly complementary to the D3R effort, as the simpler systems can probe specific aspects of the calculations with considerable precision.

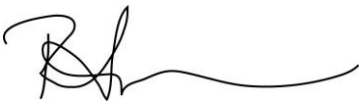
Indeed, our efforts are already strongly aligned. Thus, as you know, in 2015-2016, the D3R helped organize the SAMPL5 challenge by coordinating submission of blind predictions for both SAMPL and D3R challenges, and by integrating presentation and discussion of SAMPL and D3R challenges in the March 2016 workshop we held at UC San Diego. The workshop was a tremendous success, as documented by the anonymous post-meeting survey, and it was clear that the SAMPL challenge played an important role in what was learned.

Thus, we are enthusiastic about continuing to cooperate and coordinate, in order to minimize duplication of effort and maximize value to the computational chemistry community. In particular, we look forward to

- co-organizing and co-hosting workshops and webinars centered on SAMPL and D3R challenges
- handling submissions for the SAMPL challenges
- advertising SAMPL challenges by the same channels (*e.g.*, email lists and Twitter) used for D3R
- work together on the science so that the SAMPL and D3R together advance the technology of computer-aided drug design to the maximum possible extent

We wish you the best of luck with your proposal!

Sincerely yours,



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